The metal–insulator transition in disordered systems: a new approach to the critical behaviour

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Abstract. In the most popular approach to the numerical study of the Anderson metal–insulator transition the transfer matrix method is combined with finite–size scaling ideas. This approach requires large computer resources to overcome the statistical fluctuations and to accumulate data for a sufficient range of different values of disorder or energy. In this paper we present an alternative approach in which the basic transfer matrix is extended to calculate the derivative with respect to disorder. By so doing we are able to concentrate on a single value of energy or disorder and, potentially, to calculate the critical behaviour much more efficiently and independently of the assumed range of the critical regime. We present some initial results which illustrate both the advantages and the drawbacks of the method.

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1. Introduction

The Anderson (1958) transition in three–dimensional electronic systems has been extensively studied over recent years (Kramer & MacKinnon 1993). It is well known that increasing the fluctuations of the random potential in three–dimensional systems (3D) causes a transition from metal to insulator. This transition occurs due to a change in the nature of the electron wavefunctions under the influence of the disorder. In the insulating phase the magnitude of the potential fluctuations is sufficiently large to localise the wavefunctions to a region of space. As the disorder is reduced below a critical value the electron states become delocalised allowing conduction through the system. In models of disordered systems such as the Anderson Hamiltonian this change can be measured numerically by observing the change in the decay length of the transmission probability (the correlation length ξ) using the transfer matrix method (MacKinnon & Kramer 1981, MacKinnon 1994). Since the development (Abrahams et al. 1979) of a scaling theory for the zero–temperature dc conductance of disordered electronic systems much numerical work has focused on calculating the critical exponent for the correlation length (MacKinnon & Kramer 1981, MacKinnon 1994, Slevin & Ohtsuki 1997, Slevin & Ohtsuki 1999).

The assumption of one–parameter scaling implies that the renormalised length $\Lambda_1 = \xi_1/M$ should follow the scaling equation:

$$\frac{\mathrm{d}\ln\Lambda_1}{\mathrm{d}\ln M} = \chi_1(\ln\Lambda_1) \tag{1}$$

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with solutions of the form $\Lambda_1 = f_1(M/\xi_\infty)$. When plotted against disorder, W, for different sizes, M, the curves, f_1, all cross at a fixed point $\chi_1 = 0$ corresponding to the metal–insulator transition. ξ_∞ is the correlation length for the infinite system which diverges close to the critical point, W_c, as $\xi_\infty \sim \mid W - W_\mathrm{c} \mid^{-\nu}$. Near the critical point the scaling equation can be linearised:

$$\Lambda_1 = \Lambda_{1,\mathrm{c}} + a(W - W_\mathrm{c})M^{\frac{1}{\nu}}. \tag{2}$$

The standard method of calculating the critical exponent ν is to analyse the finite size scaling in terms of this equation. However, taking the logarithm of the derivative with respect to disorder gives us:

$$\ln\left(\left.\frac{\mathrm{d}\Lambda_1}{\mathrm{d}W}\right|_{W_\mathrm{c}}\right) = \ln a + \frac{1}{\nu}\ln M. \tag{3}$$

This expression provides a way of calculating the critical exponent from the derivative of the correlation length of the finite system Λ_1. In previous work (MacKinnon 1990) it has been noted that the calculation of the derivative $\mathrm{d}\Lambda_1/\mathrm{d}W$ would provide useful complimentary information about the scaling and a more direct approach to calculating the critical exponent. However direct estimation of the derivative has up to now been plagued by large numerical errors associated with numerical division when using a finite difference approximation $[\Lambda_1(W + \Delta W) - \Lambda_1(W)]/\Delta W$.

Our new method is an adaptation of the standard transfer matrix approach to calculate the derivative, $\dot{\mathbf{T}}$, of the transfer matrix, $\mathbf{T}$, from which it is possible to calculate the expectation value of $\mathrm{d}\Lambda_i/\mathrm{d}W$, and hence find ν. This approach is applicable for 3D cubic systems (M=L=6,8,10,12,14) rather than for quasi–1D systems. In contrast to quasi–1D systems, where the conductance is described by only one correlation length, the conductance of cubic systems is given by a sum over contribution from a series of correlation lengths. Here we present preliminary results for the scaling of each correlation length individually as well as for the conductance as a whole.

2. Computational Method

2.1. The traditional transfer matrix

The Anderson (1958) model for non–interacting electrons on a simple cubic lattice in zero magnetic field is described by the Hamiltonian:

$$H = \sum_i \epsilon_i |i\rangle\langle i| + \sum_{i \neq j} V |i\rangle\langle j|, \tag{4}$$

where $|i\rangle$ is the atomic orbital at site i, and $V = 1$ for nearest neighbours and zero otherwise. The disorder is introduced by allowing the on–site energies ϵ_i to behave stochastically. The site energies ϵ_i are chosen according to the probability distribution

$$p(\epsilon) = W^{-1}\theta(\tfrac{1}{2}W - |\epsilon|), \tag{5}$$

where θ is the step function so that $p(\epsilon)$ is a box distribution. The Schrödinger equation $H\phi = E\phi$ for a system with cross section $M \times M$ and length L can be rewritten in recursive form:

$$\begin{pmatrix} \boldsymbol{\psi}_{i+1} \\ \boldsymbol{\psi}_i \end{pmatrix} = \begin{pmatrix} E - \mathbf{H}_i & -\mathbf{1} \\ \mathbf{1} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{\psi}_i \\ \boldsymbol{\psi}_{i-1} \end{pmatrix} = \mathbf{T}_i \begin{pmatrix} \boldsymbol{\psi}_i \\ \boldsymbol{\psi}_{i-1} \end{pmatrix}, \tag{6}$$

where the $2M^2 \times 2M^2$ matrix, $\mathbf{T}$, is the so-called the transfer matrix and the $M^2 \times M^2$ matrix, $\mathbf{H}_i$ is the Hamiltonian of a single slice disconnected from the rest of the lattice. The application of $\mathbf{T}_i$ to a slice gives the solution of the Schrödinger equation for the next slice. In this way the complete wavefunction for a disordered sample of length L can be generated by repeated application of the transfer matrix:

$$\begin{pmatrix} \boldsymbol{\psi}_{L+1} \\ \boldsymbol{\psi}_L \end{pmatrix} = \prod_{i=1}^{L} \mathbf{T}_i \begin{pmatrix} \boldsymbol{\psi}_1 \\ \boldsymbol{\psi}_0 \end{pmatrix}. \tag{7}$$

The standard transfer matrix method then consists of calculating the asymptotic (i.e. $L \to \infty$) behaviour of the eigenvalues of the Hermitian matrix $\mathbf{Q}$:

$$\mathbf{Q} = \mathbf{T}^{\dagger}\mathbf{T} \tag{8}$$

by repeated orthogonalisation of the columns of $\mathbf{T}$ (MacKinnon & Kramer 1983). Alternatively, for a finite L, a system in Landauer (1970) geometry, i.e. embedded between perfectly ordered leads, may be represented in the form

$$\mathbf{Q} = \mathbf{U}^{\dagger} \left[\prod_{i=1}^{L} \mathbf{T}_i \right]^{\dagger} \mathbf{\Lambda} \mathbf{U}^{*} \mathbf{U}^{\mathrm{T}} \mathbf{\Lambda} \left[\prod_{i=1}^{L} \mathbf{T}_i \right] \mathbf{U} \tag{9}$$

where the columns (rows) of $\mathbf{U}$ ($\mathbf{U}^T\mathbf{\Lambda}$) are the right (left) eigenvectors which diagonalise $\mathbf{T}$ in the absence of disorder and

$$\mathbf{\Lambda} = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix}. \tag{10}$$

The correlation lengths ξ_i, from which the scaling properties are calculated, are related to the eigenvectors $|z_i>$ of $\mathbf{Q}$ by

$$\mathbf{Q}|z_i> = \exp(z_i)|z_i> \qquad \text{where} \quad z_i = 2\alpha_i L = 2L/\xi_i \tag{11}$$

for $i = 1, 2, ...2M^2$. In the quasi 1D limit the α_i are called Lyapunov exponents.

The normalised eigenvectors for the system with zero disorder can be grouped together to form a $2M^2 \times 2M^2$ matrix, $\mathbf{U}$, in which first M^2 columns are made from the $2M^2 \times M^2$ sub–matrix ($\mathbf{U}_+$) of eigenvectors representing waves travelling in the positive z–direction, and the last M^2 columns from those travelling in the opposite direction, ($\mathbf{U}_-$). The set of left–handed eigenvectors is given by $\mathbf{U}^{\mathrm{T}}\mathbf{\Lambda}$. The eigenvectors can be used to transform the real–space transfer matrix (6) into the wave representation:

$$\mathbf{T}_{\mathrm{w}} = \mathbf{U}^{\mathrm{T}}\mathbf{\Lambda}\mathbf{T}_L\mathbf{U}, \tag{12}$$

where $\mathbf{T}_L$ is the real–space transfer matrix for a system of length L. The transfer matrix in the wave representation, $\mathbf{T}_{\mathrm{w}}$, can be expressed in terms of the transmission and reflection matrices:

$$\mathbf{T}_{\mathrm{w}} = \begin{pmatrix} \mathbf{t} - \mathbf{r}'(\mathbf{t}')^{-1}\mathbf{r} & \mathbf{r}'(\mathbf{t}')^{-1} \\ -(\mathbf{t}')^{-1}\mathbf{r} & (\mathbf{t}')^{-1} \end{pmatrix}. \tag{13}$$

This suggests that $\mathbf{r}'$ and $\mathbf{t}'$ may be calculated from the matrix products:

$$\mathbf{t}'^{-1} = \begin{pmatrix} \mathbf{0} & \mathbf{1} \end{pmatrix} \mathbf{T}_w \begin{pmatrix} \mathbf{0} \\ \mathbf{1} \end{pmatrix} = \mathbf{U}_-^T \mathbf{\Lambda} \mathbf{T}_L \mathbf{U}_- = \mathbf{U}_-^T \mathbf{\Lambda} \prod_{n=1}^{L} \mathbf{T}_n \mathbf{U}_- \tag{14a}$$

$$\mathbf{r}'\mathbf{t}'^{-1} = \begin{pmatrix} \mathbf{1} & \mathbf{0} \end{pmatrix} \mathbf{T}_w \begin{pmatrix} \mathbf{0} \\ \mathbf{1} \end{pmatrix} = \mathbf{U}_+^T \mathbf{\Lambda} \mathbf{T}_L \mathbf{U}_- = \mathbf{U}_+^T \mathbf{\Lambda} \prod_{n=1}^{L} \mathbf{T}_n \mathbf{U}_-. \tag{14b}$$

2.2. Stabilisation of the Iteration

In practice the repeated multiplications of the matrix $\mathbf{U}_-$ by successive transfer matrices gives rise to numerical instabilities that require attention. The matrix gradually becomes dominated by the largest eigenvalues and the smaller ones are lost owing to the finite accuracy of the numerical process. It is these eigenvalues that are needed when the inverse is taken to calculate $\mathbf{t}'$. To avoid losing them the algorithm must be modified. After about ten iterations, and well before the small eigenvalues are lost, the relevant information is 'stored' by multiplying from the right by a stabilising matrix, $\mathbf{Y}$:

$$\prod_{n=1}^{10} \mathbf{T}_n \mathbf{U}_- \mathbf{Y} = \mathbf{Z}\mathbf{Y} \tag{15}$$

The matrix $\mathbf{Y}$ may be chosen to be the inverse of the top half of the $\mathbf{Z}$ (or the upper triangular matrix which orthonormalises the columns of $\mathbf{Z}$):

$$\mathbf{Z}\mathbf{Y} = \begin{pmatrix} \mathbf{Y}^{-1} \\ \mathbf{G} \end{pmatrix} \mathbf{Y} = \begin{pmatrix} \mathbf{1} \\ \mathbf{G}\mathbf{Y} \end{pmatrix}. \tag{16}$$

This process of multiplying by the inverse matrix is repeated approximately every ten iterations. The product of the $\mathbf{Y}$ is stored separately and is used at the end to solve for the reflection/transmission coefficients. Applying this method to equations (14*a*) and (14*b*) results in the following relations:

$$\mathbf{t}'^{-1}\mathbf{Y} = \mathbf{A}, \tag{17a}$$

$$\mathbf{r}'\mathbf{t}'^{-1}\mathbf{Y} = \mathbf{B}, \tag{17b}$$

where the matrices $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{Y}$ are known. The numerically stable solutions are:

$$\mathbf{t}' = \mathbf{Y}\mathbf{A}^{-1}, \tag{18a}$$

$$\mathbf{r}' = \mathbf{B}\mathbf{A}^{-1}, \tag{18b}$$

2.3. Calculating the derivatives

Our new approach extends the transfer matrix method to calculate $\dot{\mathbf{T}} = \mathrm{d}\mathbf{T}/\mathrm{d}W$ from which the $\mathrm{d}\xi_i/\mathrm{d}W$ can then be found. To preserve the multiplicative behaviour a larger matrix $\mathbf{K}$ is used:

$$\mathbf{K}_L = \begin{pmatrix} \mathbf{T}_L & \mathbf{0} \\ \dot{\mathbf{T}}_L & \mathbf{T}_L \end{pmatrix} = \prod_{i=1}^{L} \begin{pmatrix} \mathbf{T}_i & \mathbf{0} \\ \dot{\mathbf{T}}_i & \mathbf{T}_i \end{pmatrix} \tag{19}$$

where $\dot{\mathbf{T}}_i$ has the simple form:

$$\dot{\mathbf{T}}_i = \begin{pmatrix} \dot{\mathbf{H}}_i & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \tag{20}$$

where $\dot{\mathbf{H}}_i$ is the derivative of the Hamiltonian of slice i:

$$\dot{\mathbf{H}}_i = \frac{\mathrm{d}\mathbf{H}}{\mathrm{d}W} = \begin{pmatrix} \epsilon_1' & 0 & \dots & 0 & 0 \\ 0 & \epsilon_2' & \dots & 0 & 0 \\ \vdots & \vdots & \dots & \vdots & \vdots \\ 0 & 0 & \dots & \epsilon_{M^2-1}' & 0 \\ 0 & 0 & \dots & 0 & \epsilon_{M^2}' \end{pmatrix} \tag{21}$$

where ϵ_i' is a random number between -0.5 and 0.5 from (5). The larger size of the matrix increases the computational time required but because of the additional information contained in the derivative only one calculation per system size is needed to calculate ν, rather than many calculations over a wide range of disorders as in the standard method. The computational details of how to calculate the derivatives of g and ξ_i from $\dot{\mathsf{T}}_i$ are described in section 2. In section 3.1 preliminary results of the scaling of these quantities is presented.

This method cannot be applied to long systems (i.e. quasi–1D) because, from Osledec's theorem, we would obtain a limiting K_L matrix of eigenvalues which cannot be related back to the eigenvalues of T. A possible solution would be to stabilise T and $\dot{\mathsf{T}}$ simultaneously so that they would both lead to limiting matrices of eigenvalues. However, two different sets of vectors are required to orthogonalise T and $\dot{\mathsf{T}}$ and this creates problems at the end of the calculation when it becomes necessary to remove the stored stabilisation vectors. The only way to overcome these difficulties is to consider small cubic systems which do not need stabilising. In this work cubic systems of size $M = 6, 8, 10, 12$ were used.

In the polar decomposition the transfer matrix can be parameterised as (Mello et al. 1988):

$$\mathsf{T} = \mathsf{U}\Gamma\mathsf{V}, \tag{22}$$

$$= \begin{pmatrix} \mathbf{u}_4 & \mathbf{0} \\ \mathbf{0} & \mathbf{u}_2^\dagger \end{pmatrix} \begin{pmatrix} (\mathbf{1}+\boldsymbol{\lambda})^{1/2} & \boldsymbol{\lambda}^{1/2} \\ \boldsymbol{\lambda}^{1/2} & (\mathbf{1}+\boldsymbol{\lambda})^{1/2} \end{pmatrix} \begin{pmatrix} \mathbf{u}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{u}_3^\dagger \end{pmatrix} \tag{23}$$

where $\mathbf{u}_i$ are arbitrary $M \times M$ unitary matrices and $\boldsymbol{\lambda}$ is a real diagonal matrix with positive elements $\{\boldsymbol{\lambda}_i\}$. If time-reversal symmetry holds then $\mathbf{u}_3 = \mathbf{u}_1^T$ and $\mathbf{u}_4 = \mathbf{u}_2^T$. In this parameterisation the transmission matrix $\mathbf{t}'$ can be written as:

$$\mathbf{t}' = \mathbf{u}_3(\mathbf{1}+\boldsymbol{\lambda})^{-1/2}\mathbf{u}_2 \tag{24}$$

and the conductance as:

$$g = \mathrm{Tr}(\mathbf{t}'\mathbf{t}'^\dagger) = \mathrm{Tr}(\mathbf{u}_3(\mathbf{1}+\boldsymbol{\lambda})^{-1}\mathbf{u}_3^\dagger), \tag{25}$$

$$= \sum_{i=1}^{M} \frac{1}{1+\lambda_i} \tag{26}$$

The Lyapunov exponents for the ensemble are derived by substitution of the polar decomposition (23) in the matrix product Q (8,9)

$$Q = \begin{pmatrix} \mathbf{u}_1(\mathbf{1}+2\boldsymbol{\lambda})\mathbf{u}_1^\dagger & 2\mathbf{u}_1\sqrt{\boldsymbol{\lambda}(\mathbf{1}+\boldsymbol{\lambda})}\mathbf{u}_3 \\ 2\mathbf{u}_3^\dagger\sqrt{\boldsymbol{\lambda}(\mathbf{1}+\boldsymbol{\lambda})}\mathbf{u}_1^\dagger & \mathbf{u}_3^\dagger(\mathbf{1}+2\boldsymbol{\lambda})\mathbf{u}_3 \end{pmatrix} \tag{27}$$

Q is Hermitian positive so the eigenvalues are positive real numbers and the flux conservation constraint, $\mathsf{Q}^{-1} = \boldsymbol{\Lambda}\mathsf{Q}\boldsymbol{\Lambda}$ requires that the eigenvalues come in inverse pairs. Strictly speaking the Lyapunov exponents α_i (11) are defined only in the quasi-1D limit, but in this work we will also use the term for arbitrary L. Applying Osledec's theorem of random matrix products (Pichard & Sarma 1981*a*, Pichard & Sarma 1981*b*), the Lyapunov exponents are self–averaging for large L. Hence, taking the limit of large L is statistically equivalent to an ensemble average over many different realisations of the disorder. Computationally, for samples of width M close to the transition, convergence of the first Lyapunov exponent to 1% accuracy is achieved for a length $L \sim 10^4 \times M$. The conductance can be expressed in terms of the Lyapunov exponents (Pichard 1984):

$$g = 2\sum_{i=1}^{N} \frac{1}{1+\cosh(2L\alpha_i)} \tag{28}$$

In the quasi-1D limit ($L \gg 1$) the conductance can be written as:

$$g \sim \sum_{i=1}^{N} e^{-2\alpha_i L} = e^{-2\alpha_1 L}\left(1 + \sum_{i=2}^{N} e^{-2(\alpha_i - \alpha_1)}\right) \tag{29}$$

where the $N \sim M^{d-1}$ Lyapunov exponents are ordered and α_1 is the smallest. As the length of the system is increased the fractional contribution to the current from the higher Lyapunov exponents rapidly decreases. The conductance is dominated by the first Lyapunov exponent and the system is similar to the 1D case where there is only one Lyapunov exponent (one conductance channel) and all the states are localised. Since there are no other relevant length scales present the localisation length is equivalent to the correlation length of the finite system, ξ_1, and is defined as:

$$\frac{1}{\xi_1} = -\lim_{L\to\infty} \frac{\ln g(L)}{2L} = \lim_{L\to\infty} \alpha_1 \tag{30}$$

From the Hellman–Feynman theorem the expectation value of the derivative of the eigenvalues, τ_i, of $\mathbf{t}'^{\dagger}\mathbf{t}'$ can be calculated:

$$\frac{\mathrm{d}\tau_i}{\mathrm{d}W} = \boldsymbol{u}_i^{\dagger} \frac{\mathrm{d}\mathbf{t}'^{\dagger}\mathbf{t}'}{\mathrm{d}W} \boldsymbol{u}_i \tag{31a}$$

$$= 2\Re\left(\boldsymbol{u}_i^{\dagger}\mathbf{t}'^{\dagger}\frac{\mathrm{d}\mathbf{t}'}{\mathrm{d}W}\boldsymbol{u}_i\right), \tag{31b}$$

where $\boldsymbol{u}_i$ is the eigenvector corresponding to τ_i. To find the $\boldsymbol{u}_i$ and τ_i it is necessary to perform an initial calculation of the transfer matrix as outlined in section 2.1. Then $\boldsymbol{u}_i$ is used in a calculation of the derivative from equation (31*b*). The expectation value of the derivative is only calculated for the smallest ten Lyapunov exponents to avoid the necessity of stabilising the matrices. If the expectation value of the whole matrix was to be calculated, the smallest expectation values would rapidly become insignificant compared to the largest, and would be lost in the rounding errors. In general the expectation value for a quasi 1D system cannot be calculated because as L increases the result rapidly becomes independent of initial conditions, i.e. independent of the initial vector ϕ_i.

Starting from equation (31*b*) we derive the form used in the computational calculations. From (14*a*) we have:

$$\mathbf{t}'^{-1} = \mathbf{U}_-^{\mathrm{T}} \mathbf{\Lambda} \mathbf{T}_L \mathbf{U}_- \tag{32}$$

where $\mathbf{U}_-$ correspond to eigenvectors in the leads with negative k_z. Taking derivatives and using equation (19) we obtain:

$$\frac{\mathrm{d}\mathbf{t}'^{-1}}{\mathrm{d}W} \tag{33}$$

from the identity $\mathbf{t}'^{-1}\mathbf{t}' = 1$ we can write:

$$\frac{\mathrm{d}\mathbf{t}'}{\mathrm{d}W} = -\mathbf{t}' \frac{\mathrm{d}\mathbf{t}'^{-1}}{\mathrm{d}W} \mathbf{t}' \tag{34}$$

therefore we have:

$$\mathbf{t}'^{\dagger}\frac{\mathrm{d}\mathbf{t}'}{\mathrm{d}W} = -\mathbf{t}'\mathbf{U}_-^{\mathrm{T}}\mathbf{\Lambda}\dot{\mathbf{T}}_L\mathbf{U}_-\mathbf{t}' \tag{35}$$

where the transmission matrices come from the initial calculation and still contain the evanescent modes. Only at this point can we remove the evanescent modes (indicated by application of $\mathbf{Q}$) and calculate the expectation value:

$$\frac{\mathrm{d}}{\mathrm{d}W}(1+\lambda_i)^{-1} = -\phi_i \mathbf{Q}^{\mathrm{T}}\mathbf{t}'\mathbf{U}_-^{\mathrm{T}}\mathbf{\Lambda}\begin{pmatrix}\mathbf{0}\\ \mathbf{1}\end{pmatrix}\prod_i^{L}\mathbf{K}_i\begin{pmatrix}\mathbf{1}\\ \mathbf{0}\end{pmatrix}\mathbf{U}_-\mathbf{t}'\mathbf{Q}\phi_i \tag{36}$$

where **Q** is an $M \times M'$ matrix with all elements zero, except for $Q_{nn} = 1, 1 \leq n \leq N$ which correspond to the N non–evanescent modes. The actual computation starts with the initial vector on the right and by successive matrix products moves through to the left. The derivative of Λ_i can be calculated (Pichard 1984):

$$\frac{\mathrm{d}\Lambda_i}{\mathrm{d}W} = -4\frac{\mathrm{d}\lambda_i}{\mathrm{d}W}[\cosh^{-1}(2\lambda_i + 1))^2 \sinh(\cosh^{-1}(2\lambda_i + 1))]^{-1} \tag{37}$$

These values were found to be in agreement with the derivative as calculated from the normal method, $\approx (\Lambda_{17.5} - \Lambda_{16.5})$. The critical exponent is calculated by fitting a straight line to equation (3).

The derivative of the conductance g can be calculated from the derivative of the LE's (37). The one–parameter scaling theory is formulated in terms of the conductance and the scaling behaviour of this quantity is considered first in the next section before considering each LE individually.

3. Cubic systems

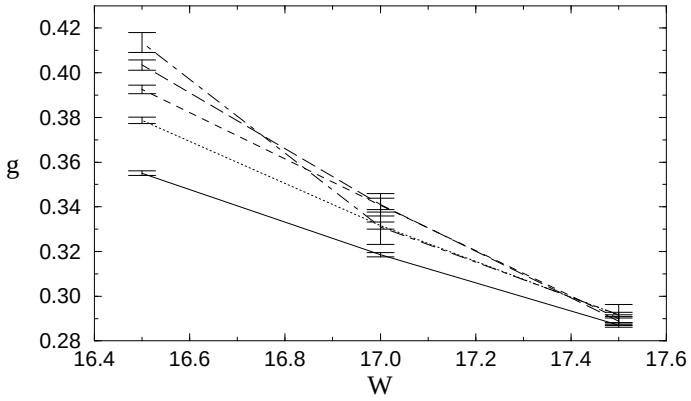

Figure 1. Conductance, g in units of e^2/h, vs. disorder, W, for $M = 6$ (——), 8 (· · · · · ·), 10 (– – –), 12 (— — —) & 14 (— · —).

3.1. Scaling of the conductance

To estimate the critical point we have plotted (figure 1) the conductance g against disorder W for system sizes $M = 6, 8, 10, 12, 14$. The value of critical disorder, W_c, is not expected to depend on the quantity being considered. Therefore, a size–independent critical point at approximately $W = 16.5$ would be anticipated to be in agreement with the values calculated from both energy statistics (Hofstetter & Schreiber 1993, Zharekeshev & Kramer 1994) of cubes and from the analysis of the 1st LE in quasi–1D systems. However, it is clear that the apparent critical disorder is above $W = 16.5$ within the error bars of the calculation. The results are also qualitatively the same for $\log(g)$. This movement of the critical point from the expected value of $W = 16.5$ is probably due to the presence of the leads connected to the ends of the cube. This is in agreement with other results (Slevin et al. 2000, Kawarabayashi et al. 2000) which find that the conductance is size dependent at $W = 16.54$ with periodic boundary conditions. However, with hard wall boundary conditions the conductance is found to be virtually size–independent at $W = 16.54$ (Slevin & Ohtsuki 1997). In energy statistics

calculations the boundary conditions affect the critical distributions but do not appear to shift the critical point (Braun & Pascaud 1998).

Table 1. At disorder $W = 16.5$ the number of iterations, open modes and the 1st LE for cubic samples , $E = 0$.

M	iterations	modes	Λ_1
6	100000	21	0.671 ± 0.0015
8	50000	45	0.694 ± 0.002
10	30000	61	0.709 ± 0.003
12	20000	95	0.718 ± 0.003
14	5000	123	0.729 ± 0.007

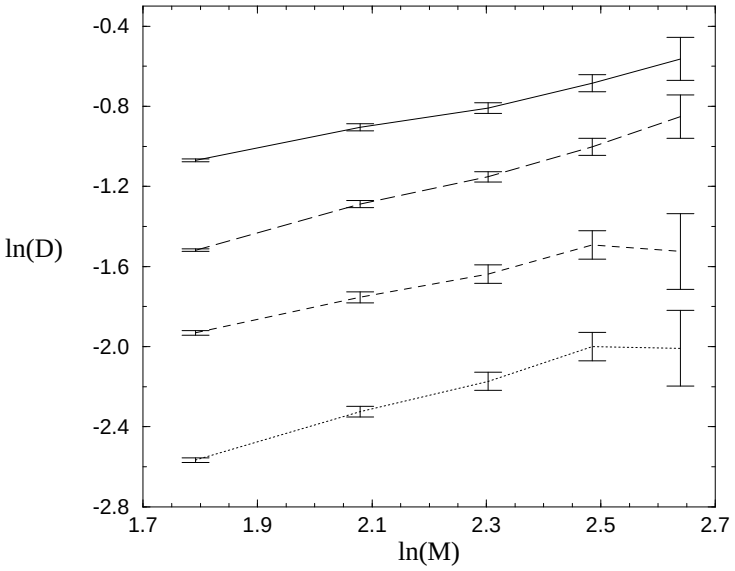

Figure 2. $\ln D$ vs. $\ln M$ for $W = 16.5$ and $M = 6, 8, 10, 12, 14$. The gradient is equal to $1/\nu$. $D = \langle \mathrm{d}\log(g)/\mathrm{d}W\rangle$ (——), $\langle \mathrm{d}\log(g)/\mathrm{d}W\rangle$ / $\langle\log(g)\rangle$ (— — —), $\langle \mathrm{d}g/\mathrm{d}W\rangle$ / $\langle g\rangle$ (– – –), $\langle \mathrm{d}g/\mathrm{d}W\rangle$ (· · · · · ·).

Applying equation (3) with g as the scaling parameter gives us:

$$\ln(D) = b + \frac{1}{\nu}\ln M \tag{38}$$

with $D = \mathrm{d}g/\mathrm{d}W|_{W_\mathrm{c}}$. If $\log g$ is used as the scaling parameter then $D = 1/g\ \mathrm{d}g/\mathrm{d}W|_{W_\mathrm{c}}$. Also considered were $D = \langle \mathrm{d}g/\mathrm{d}W|_{W_\mathrm{c}}\rangle/\langle g\rangle$ and $D = \langle \mathrm{d}\log(g)/\mathrm{d}W|_{W_\mathrm{c}}\rangle/\langle\log(g)\rangle$. The plot of equation (38) is given in figure 2 and the critical exponent found by a 'least–squares–fit' of the gradient is given in table 2. The error in the value of g is considerably smaller than the error in the gradient and can be ignored when calculating the standard deviation of the fit. From the error bars on the graph we can see that $\log(g)$ produces slightly more accurate results because it decreases the influence of the infrequent but very large values of the derivative. The $M = 14$ data is not used in the calculation of the critical exponents. The results from the same calculation performed at $W_\mathrm{c} = 17.5$ are also given in table 2. On average the critical exponents appear to be slightly lower in value for $W_\mathrm{c} = 17.5$. Clearly the

Table 2. Critical exponents calculated from the conductance of cubes with sizes $M = 6, 8, 10, 12$

W	D	ν	χ^2	Q
16.5	$\frac{\mathrm{d}\log(g)}{\mathrm{d}W}$	1.85 ± 0.12	0.7	0.7
16.5	$\left\langle \frac{\mathrm{d}\log(g)}{\mathrm{d}W} \right\rangle / \langle \log(g) \rangle$	1.34 ± 0.066	1.0	0.6
16.5	$\frac{\mathrm{d}g}{\mathrm{d}W}$	1.24 ± 0.095	0.3	0.9
16.5	$\left\langle \frac{\mathrm{d}g}{\mathrm{d}W} \right\rangle / \langle g \rangle$	1.65 ± 0.17	0.2	0.9
17.5	$\frac{\mathrm{d}\log(g)}{\mathrm{d}W}$	1.34 ± 0.073	1.4	0.5
17.5	$\left\langle \frac{\mathrm{d}\log(g)}{\mathrm{d}W} \right\rangle / \langle \log(g) \rangle$	1.30 ± 0.068	1.2	0.5
17.5	$\frac{\mathrm{d}g}{\mathrm{d}W}$	1.23 ± 0.14	0.4	0.8
17.5	$\left\langle \frac{\mathrm{d}g}{\mathrm{d}W} \right\rangle / \langle g \rangle$	1.28 ± 0.15	0.3	0.9

observed shift of the critical point is completely independent of our new method to calculate the critical exponent. However this deviation from scaling theory may well be prejudicing the critical exponent obtained from the new method. Nevertheless there is general agreement with previous calculations of the critical exponent which give a value of $\nu \approx 1.5$.

There are thus two deviations from the expected results, both of which are probably due to finite size effects: the shift in the apparent critical disorder and the dependence of the calculated exponent on the particular average of g used. However, another possible factor is the properties of the leads for which the number of open channels represents an additional degree of freedom. This requires further investigation.

3.2. Scaling of the Lyapunov exponents

For cubic systems attached to leads the contribution of the 1st 'Lyapunov exponent' § to the value of the conductance in the critical region can be calculated. At $W = 16.5$ the 1st LE makes up 85% of the conductance and approximately 74% of the derivative of the conductance. Therefore the higher Lyapunov exponents do have physical meaning even though the dominant contribution is from the 1st exponent. Scaling higher Lyapunov exponents is analogous to scaling energy statistics at large energy scales (such as $P(i, s)$ for large i) (Taylor 1998), since both correspond to short length scale events.

The 1st LE is plotted against disorder in figure 3. Within the error bars of the calculation it can be concluded that the critical point is above $W = 16.5$ as was the case with the conductance g. This shift of the critical point is even clearer in the more accurate data for the 6th LE (figure 3). Qualitatively similar results occur for $\langle \Lambda_i \rangle$.

In figure 4 equation (3) is plotted with $D = \left\langle \mathrm{d}\Lambda_i^{-1}/\mathrm{d}W \right\rangle$ for $W = 16.5$, i.e. the first

§ The Lyapunov exponents α_i are strictly defined only in the quasi–1D limit but in this work the definition is extended to include arbitrary L (11).

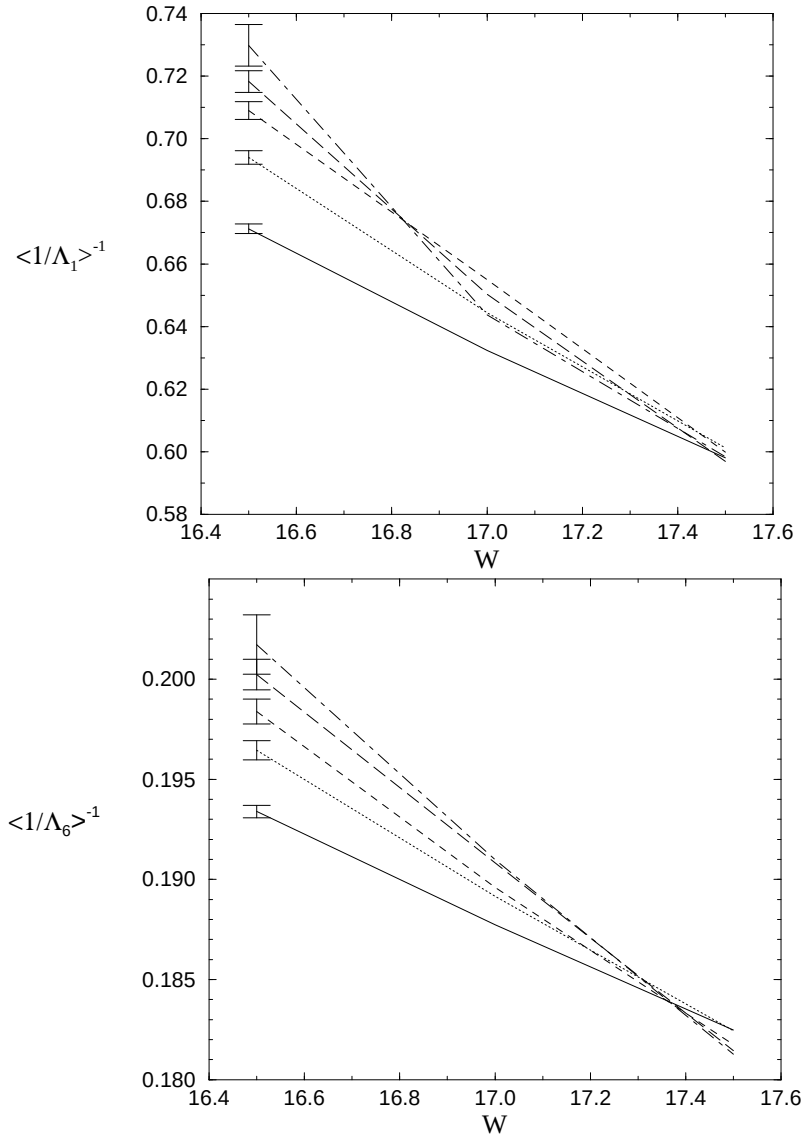

Figure 3. Dependence of $\langle \Lambda_1 \rangle$ (upper figure) and $\langle \Lambda_6 \rangle$ (lower figure) on disorder W for cubic systems of size M. Data points at $W = 16.5, 17.0, 17.5$. $M = 6$ (——), 8 (· · · · · ·), 10 (– – –), 12 (— — —), & 14 (— · —).

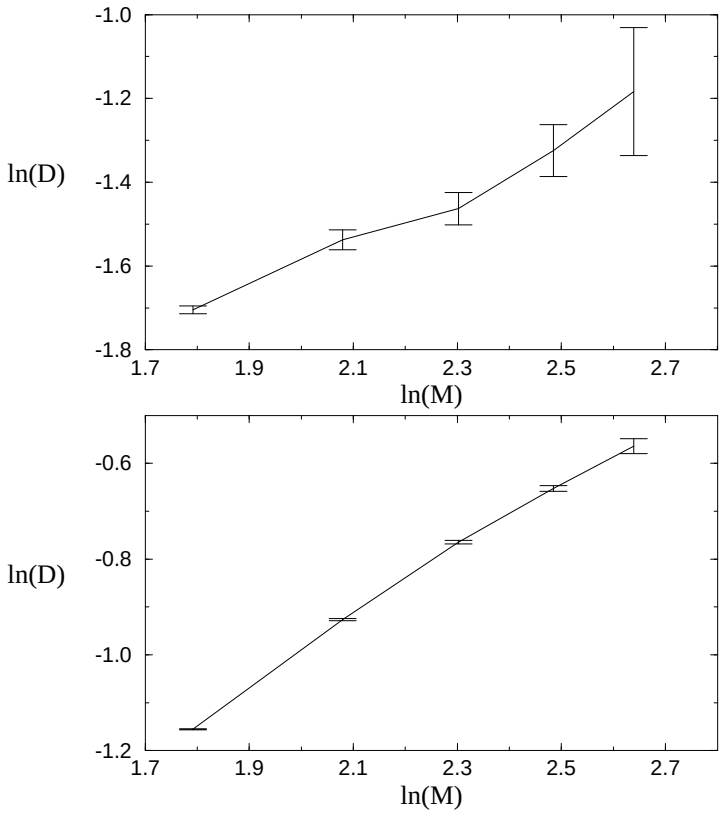

Figure 4. Scaling of the Lyapunov exponents. Slope is equal to $1/\nu$. $D = \left\langle \mathrm{d}\Lambda_i^{-1}/\mathrm{d}W \right\rangle$ at $i = 1$ (upper figure), $i = 6$ (lower figure).

LE, $\left\langle \Lambda^{-1} \right\rangle$, is being scaled.

From one parameter scaling the gradient of this line is equal to the inverse of the critical exponent.

The accuracy of the data increases when we consider higher LE's and the result for the 6th LE is shown in figure 4. In theory this should be a straight line but the accuracy of the data is high enough to observe a definite curvature indicating deviations from one–parameter scaling theory. Although the curve can be fitted by a straight line the quality–of–fit measure χ^2 is too large (and $Q \ll .1$) which indicates the curvature cannot be ignored. At $W = 17.5$, which is nearer the apparent critical point (figure 5), the results are qualitatively the same and the curvature in the $\ln(D)$ vs $\ln(M)$ plot is again observed for the higher Lyapunov exponents. This type of curvature indicates that scaling corrections exist for the gradient. A full analysis in terms of this equation was not possible because the number of data points is too small to obtain sufficient accuracy. In future studies with a full compliment of data from $M = 4$ to 14 it is possible that the functional form of the corrections could be found and subtracted to obtain a crossing at $W = 16.5$. It is impossible to tell if the curvature also exists for the 1st LE because it could be masked by the larger error bars of the data.

The results of the straight line fit to calculate the critical exponent are given in figure 6. As mentioned, although the critical exponents calculated from the higher Lyapunov exponents are more accurate the χ^2 becomes too large. However the fits illustrate that the scaling

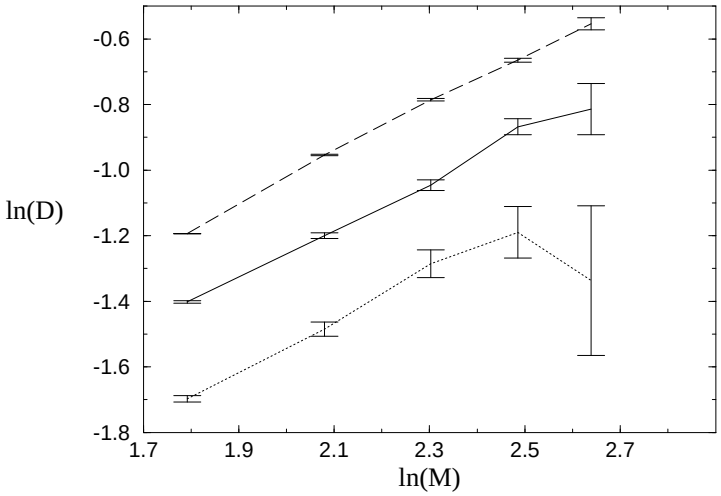

Figure 5. Scaling of the 1st(· · · · · ·), 2nd(——) and 6th(– – –) Lyapunov exponents. Slope is equal to $1/\nu$. $D = \langle \mathrm{d}(1/\Lambda_i)/\mathrm{d}W \rangle$, $W = 17.5$

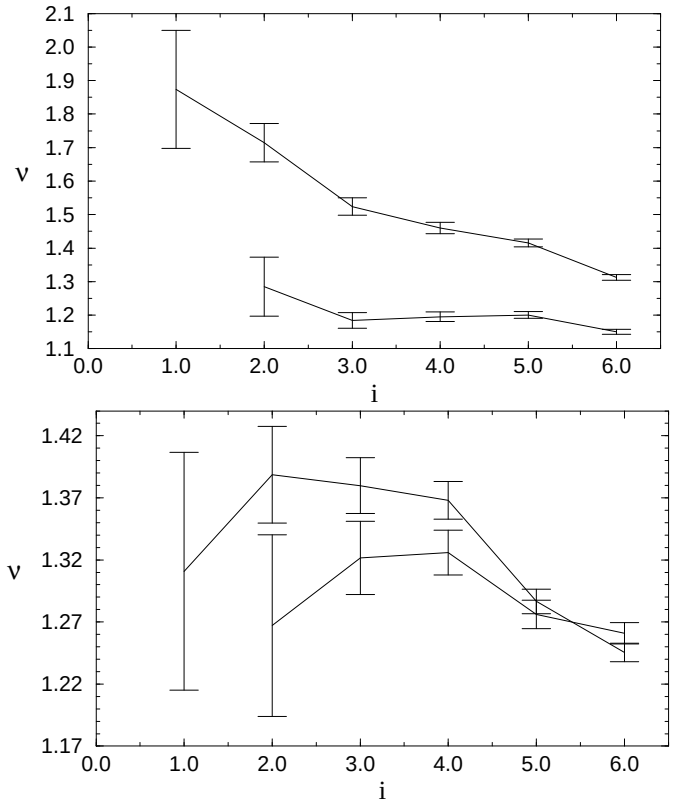

Figure 6. Critical exponents calculated from $1/\Lambda_i$ (higher curve) and from Λ_i (lower curve) for $i = 1 - 6$. $W = 16.5$ (upper figure), $W = 17.5$ (lower figure)

behaviour is approximately in agreement with previously calculated values of the critical exponent.

4. Conclusions

We have introduced a new approach to calculating the critical behaviour of the Anderson transition in disordered systems, which has the potential to overcome some of the numerical difficulties which have plagued such calculations in the past. As the method is only requires a calculation at a single value of disorder it eliminates the difficulties associated with the necessity of fitting to a range of values of disorder and the associated uncertainties associated with the determination of the range of disorder over which the critical behaviour is valid. The initial results are promising, although the necessity of working with cubes rather than long systems introduces deviations from the expected behaviour. We expect these deviations to be explicable in terms of the usual corrections to scaling (Slevin & Ohtsuki 1997, Slevin & Ohtsuki 1999, Ohtsuki et al. 1999, Slevin & Ohtsuki 2001).

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References

Abrahams E, Anderson P W, Licciardello D C & Ramakrishnan T V 1979 *Phys. Rev. Lett.* **42**, 673.
Anderson P W 1958 *Phys. Rev.* **109**, 1492.
Braun, D Mountambaux G & Pascaud M 1998 *Phys. Rev. Lett.* **81**, 1062.
Hofstetter E & Schreiber M 1993 *Europhys. Lett.* **21**, 933.
Kawarabayashi T, Ohtsuki T & Slevin K M 2000 *Physica B* **284-288**, 1549.
Kramer B & MacKinnon A 1993 *Rep. Prog. Phys.* **56**, 1469.
Landauer R 1970 *Phil. Mag.* **21**, 863.
MacKinnon A 1990 *in* F Kuchar, H Heinrich & G Bauer, eds, 'Localization and Confinement of Electrons in Semiconductors' Vol. 97 of *Springer Ser. Sol. St. Sci.* Springer Heidelberg p. 111.
MacKinnon A 1994 *J. Phys. Condensed Matter* **6**, 2511.
MacKinnon A & Kramer B 1981 *Phys. Rev. Lett.* **47**, 1546.
MacKinnon A & Kramer B 1983 *Z. Physik* **B53**, 1.
Mello P A, Pereyra P & Kumar N 1988 *Annals of Physics* **181**, 290.
Ohtsuki T, Slevin K & Kawarabayashi T 1999 *Annalen der Physik* **8**, 655.
Pichard J L 1984 PhD thesis Université de Paris Orsay.
Pichard J L & Sarma G 1981*a J. Phys. C: Solid State Physics* **14**, L127.
Pichard J L & Sarma G 1981*b J. Phys. C: Solid State Physics* **14**, L617.
Slevin K M & Ohtsuki T 1997 *Phys. Rev. Lett.* **78**, 4083.
Slevin K M & Ohtsuki T 1999 *Phys. Rev. Lett.* **82**, 382.
Slevin K M, Ohtsuki T & Kawarabayashi T 2000 *Phys. Rev. Lett.* **84**, 3915.
Slevin K & Ohtsuki T 2001 *Phys. Rev.* **B63**, 045108/1.
Taylor A P 1998 The statistics of quantum transport through disordered systems PhD thesis University of London. *http://www.cmth.ph.ic.ac.uk/research/theses/A.P.Taylor.pdf
Zharekeshev I K & Kramer B 1994 *Phys. Rev.* **51**, 17239.